

# Normal Equation, Data Fitting, and QR

## 1 APPROXIMATE SOLUTIONS OF A MATRIX EQUATION.

For the equations  $Ax = \mathbf{b}$  below, write the normal equation and then use it to find the best approximate solution  $\hat{\mathbf{x}}$ . For extra understanding, check if  $\hat{\mathbf{x}}$  is actually also a solution to the original equation.

$$\begin{array}{llll}
 \text{(a)} \begin{bmatrix} 2 \\ 3 \end{bmatrix} [x] = \begin{bmatrix} 4 \\ 6 \end{bmatrix} & \text{(c)} \begin{bmatrix} 1 & -2 \\ 2 & -4 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 3 \\ 6 \end{bmatrix} & \text{(e)} \begin{bmatrix} 1 & 0 \\ 1 & -1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} & \text{(f)} \begin{bmatrix} 1 & -1 \\ 1 & 0 \\ 1 & 1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} -1 \\ 2 \\ 0 \\ 1 \end{bmatrix} \\
 \text{(b)} \begin{bmatrix} 2 \\ 3 \end{bmatrix} [x] = \begin{bmatrix} 1 \\ 8 \end{bmatrix} & \text{(d)} \begin{bmatrix} 1 & -2 \\ 2 & -4 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 2 \\ 1 \end{bmatrix} & & 
 \end{array}$$

## 2 LEAST SQUARES DATA FITTING USING THE NORMAL EQUATION.

For the following data sets and the function  $f(t)$ ,

- (i) write a matrix equation  $Ax = \mathbf{b}$  to compute the coefficients of  $f(t)$ ,
- (ii) write the associated normal equation  $A^T A \hat{\mathbf{x}} = A^T \mathbf{b}$ ,
- (iii) solve for the best approximate solution for the coefficients of  $f(t)$  and write  $\hat{f}(t)$

$$\begin{array}{lll}
 \text{(a)} f(t) = a & \text{(b)} f(t) = bt & \text{(c)} f(t) = a + bt \\
 \begin{array}{c|c|c|c|c} t & -1 & 0 & 1 & 2 \\ \hline f(t) & -3 & -1 & 1 & 0 \end{array} & \begin{array}{c|c|c|c|c} t & -1 & 0 & 1 & 2 \\ \hline f(t) & -3 & -1 & 1 & 0 \end{array} & \begin{array}{c|c|c|c|c} t & -1 & 0 & 1 & 2 \\ \hline f(t) & -3 & -1 & 1 & 0 \end{array} \\
 \text{(d)} f(t) = a + bt^2 & \text{(e)} f(t) = a + b/t & \text{(f)} f(t) = a \cos(t) + b \cos(2t) \\
 \begin{array}{c|c|c|c|c} t & -1 & 0 & 1 & 2 \\ \hline f(t) & -3 & 1 & 1 & -1 \end{array} & \begin{array}{c|c|c|c} t & 1/3 & 1/2 & 1 \\ \hline f(t) & 3 & 0 & -6 \end{array} & \begin{array}{c|c|c|c|c} t & 0 & \pi/2 & \pi & 3\pi/2 \\ \hline f(t) & 1 & -1 & 3 & 2 \end{array}
 \end{array}$$

## 3 USING SCALED QR-DECOMPOSITION

Use the scaled QR-decompositions given below to solve.

$$\begin{array}{ll}
 \text{(a)} \begin{bmatrix} 2 & 1 & -2 \\ 1 & 2 & 2 \\ 2 & -2 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & -1 \\ 0 & 2 & 1 \\ 0 & 0 & 3 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -3 \\ 9 \\ 3 \end{bmatrix} & \text{(b)} \begin{bmatrix} 2 & 1 & 4 \\ 1 & 1 & -5 \\ -3 & 1 & 1 \end{bmatrix} \begin{bmatrix} 2 & 2 & -3 \\ 0 & 2 & -4 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 1 \\ 8 \\ -2 \end{bmatrix} \\
 \text{(c)} \begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & -1 & 0 \\ 1 & 0 & -1 \end{bmatrix} \begin{bmatrix} 1 & 2 & -3 \\ 0 & 2 & -1 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 3 \\ 5 \\ 1 \\ -1 \end{bmatrix} & \text{(d)} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 2 & -2 & 0 \\ 2 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 2 & 3 \\ 0 & 1 & 2 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 4 \\ 0 \\ 8 \\ 5 \end{bmatrix}
 \end{array}$$

## 4 COMPUTING SCALED QR-DECOMPOSITION

Compute a scaled QR decompositions for the matrices below.

$$\begin{array}{llll}
 \text{(a)} \begin{bmatrix} 1 & 2 & 3 \\ 1 & 0 & -9 \\ 2 & 5 & -3 \end{bmatrix} & \text{(b)} \begin{bmatrix} 1 & -1 & 8 \\ 2 & -7 & 6 \\ 2 & -6 & -1 \end{bmatrix} & \text{(c)} \begin{bmatrix} 2 & -8 & 11 \\ 3 & 7 & -3 \\ -5 & 1 & -5 \end{bmatrix} & \text{(d)} \begin{bmatrix} -9 & -7 & 8 \\ 7 & 10 & -9 \\ 1 & -2 & 4 \end{bmatrix} \\
 \text{(e)} \begin{bmatrix} 1 & 5 & 4 \\ 1 & -1 & -10 \\ 1 & 5 & 0 \\ 1 & 3 & -2 \end{bmatrix} & \text{(f)} \begin{bmatrix} 1 & 4 & 0 \\ 1 & 3 & 3 \\ 1 & 2 & 4 \\ 1 & 3 & 1 \end{bmatrix} & \text{(g)} \begin{bmatrix} 1 & 5 & -7 \\ 1 & 7 & 7 \\ 2 & 7 & -5 \\ 2 & 7 & -5 \end{bmatrix} & \text{(h)} \begin{bmatrix} 1 & -1 & 5 \\ 2 & -7 & 1 \\ 2 & -4 & 9 \\ 2 & -8 & -6 \end{bmatrix}
 \end{array}$$

## 5 MATLAB

- Recall that transpose in MatLab is `'`. To solve the normal equation it is fastest enter A and b first and then use the command  $(A' * A) \setminus (A' * b)$  to divide  $A^T A \hat{x} = A^T b$ .

**Example.** Find the best approximate solution to the matrix equation 
$$\begin{bmatrix} 1 & -1 \\ 1 & 0 \\ 2 & 3 \\ -1 & 5 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} -1 \\ 7 \\ -2 \\ 3 \end{bmatrix}$$

```
1 >> A = [1 -1; 1 0; 2 3; -1 5]
2 >> b = [-1; 7; -2; 3]
3 >> x_hat = (A' * A) \ (A' * b)
```

In this case the error vector is given by

```
4 >> e = b - A * x_hat
```

with squared error

```
5 >> e' * e
```

- It is slightly faster to enter column vectors into MatLab as transposes of row vectors. The same trick works for matrices that don't have many columns. For example lines 1 and 2 above could be replaced by

```
1 >> A = [1 1 2 -1; -1 0 3 5] '           % A = [1 -1; 1 0; 2 3; -1 5]
2 >> b = [-1 7 -2 3] '                 % b = [-1; 7; -2; 3]
```

- To solve data fitting problems using MatLab, we first enter the independent variable `t`, then we build the matrix A, column by column, plugging `t` into the terms multiplied by unknown constants.

**Example.** Fit the formula  $f(t) = a + bt + ct^2$  to the data

$t$	-1	0	1	2	3	4
$f(t)$	-3	1	1	-1	-6	-8

```
6 >> t = [-1 0 1 2 3 4] '           % column vector of t-values
7 >> A = [t.^0 t.^1 t.^2]           % matrix of [ 1 t t^2 ]
8 >> f = [-3 1 1 -1 -6 -8] '       % column vector of f-values
9 >> coeff = (A' * A) \ (A' * f)    % normal eqn for A * coeff = f
```

Line 7 uses `t.^2` instead of `t^2` to tell MatLab to square `t` **element-wise** rather than square `t` as a **matrix**. Without the `.` MatLab would have returned an error, since you cannot multiply two 6x1 matrices.

- MatLab has a command `qr` which gives the (unscaled) QR-decomposition. The (unscaled) QR decomposition differs from our version by insisting that all columns of Q have length 1. In practice this means dividing each column of Q by its length and multiplying the corresponding rows of R by this length.

We can write MatLab code to compute scaled QR decomposition using a `for` loop to build Q column by column. Begin with Q = first column of A, and then convert the other columns of A to be columns of Q by computing error vectors for the approximate solution to  $Qx =$  (next column of A).

**Example.** Compute the scaled QR decomposition of  $A = \begin{bmatrix} 1 & 4 & 11 \\ 2 & 6 & -9 \\ 2 & 1 & -10 \end{bmatrix}$ .

```
10 >> A = [1 4 11; 2 6 -9; 2 1 -10]    % Enter matrix A
11 >> Q = A(:,1)                       % Begin with Q = col 1 of A
12 >> R = [1 0 0; 0 1 0; 0 0 1]        % Begin with R = identity matrix
13 >> for (col = 2:size(A,2))          % Loop over columns of A
14     x_hat = (Q' * Q) \ (Q' * A(:,col)) % Normal eqn for Q x = (next col)
15     e = A(:,col) - Q * x_hat         % Error vector for x_hat
16     Q = [Q e]                       % Error vector is next col of Q
17     R(1:col,col) = x_hat             % x_hat is next col of R
18 end                                 % End of loop
```

Line 13 uses the command `size(A,2)` to get the number of columns of A. The command `size(A,1)` gives the number of rows of A, and the command `size(A)` gives the number of rows and columns.